

# Analytical Solution for the Size of the Minimum Dominating Set in Complex Networks

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## Abstract

Domination is the fastest-growing field within graph theory with a profound diversity and impact in real-world applications, such as the recent breakthrough approach that identifies optimized subsets of proteins enriched with cancer-related genes. Despite its conceptual simplicity, domination is a classical NP-complete decision problem which makes analytical solutions elusive and poses difficulties to design optimization algorithms for finding a dominating set of minimum cardinality in a large network. Here we derive for the first time an approximate analytical solution for the density of the minimum dominating set (MDS) by using a combination of cavity method and Ultra-Discretization (UD) procedure. The derived equation allows us to compute the size of MDS by only using as an input the information of the degree distribution of a given network.

## INTRODUCTION

The research on complex networks in diverse fields [1, 2], based on applied graph theory combined with computational and statistical physics methods, has experienced a spectacular growth in recent years and has led to the discovery of ubiquitous patterns called scale-free networks [3], unexpected dynamic behavior [4], robustness and vulnerability features [5–7], and applications in natural and social complex systems [1, 2]. On the other hand, domination is an important problem in graph theory which has rich variants, such as independence, covering and matching [8]. The mathematical and computational studies on domination have led to abundant applications in disparate fields such as mobile computing and computer communication networks [9], design of large parallel and distributed systems [10], analysis of large social networks [11–13], computational biology and biomedical analysis [14] and discrete algorithms research [8].

More recently, the Minimum Dominating Set (MDS) has drawn the attention researchers to controllability in complex networks [15–17], to investigate observability in power-grid [18] and to identify an optimized subset of proteins enriched with essential, cancer-related and virus-targeted genes in protein networks [19]. The size of MDS was also investigated by extensively analysing several types of artificial scale-free networks using a greedy algorithm in [20]. The problem to design complex networks that are structurally robust has also recently been investigated using the MDS approach [21, 22].

Despite its conceptual simplicity, the MDS is a classical NP-complete decision problem in computational complexity theory [23]. Therefore, it is believed that there is no a theoretically efficient (i.e., polynomial time) algorithm that finds an exact smallest dominating set for a given graph. It is worth noticing that although it is an NP-hard problem, recent results have shown that we can use Integer Linear Programming (ILP) to find optimal solution [15, 19, 21]. Moreover, for specific types of graph such a tree (i.e., no loops) and even partial- $k$ -tree, it can be solved using Dynamic Programming (DP) in polynomial time [24].

Especially, the density (or fraction) of MDS, defined as the size of MDS versus the total number of nodes in a network, is important to estimate the cost-efficient network deployment of controllers. It is less expensive to have ten power plants operating as controllers in a large network of 1,000 sites than one hundred. Similarly, acting on two protein targets via drug interactions is always better than acting on ten protein targets to minimize adverse side

effects. Although we can use an ILP method for obtaining an MDS and the density of MDS, we do not have an analytic solution for the density of MDS. Note that even though optimal solution for MDS can be found using ILP method, this kind of technique is very generic and operates as a *black box* so that its systematic application does not provide us any knowledge about the details of the particular problem under study. Moreover, from a physical point of view, analytic solutions always enable us to have a deeper understanding of the problem by examining dependences with other variables. Here, we derive for the first time an analytical solution for an MDS by using cavity method.

Cavity method is a well-known methodology developed by physicists working on statistical mechanics (e.g. spin glasses [25]). However, this technique has also been extended and applied to non-physical systems, including network theory in which nodes can be abstracted to some extent. For example, applications include the analysis of random combinatorial problems such as weighted matching [26], the vertex cover [27] and the travelling salesman problem [28]. Moreover, recently cavity method was used to determine the number of matchings in random graphs [29], the maximal independent sets [30], the random set packing [31] and the minimum weight Steiner tree [32] and controllability using maximum matching [33], extending the work done in [29] for undirected networks to directed networks.<sup>1</sup> It is also well-known that cavity method computed at zero temperature limit has been applied to networks and used in many works, which have led to derive elegant analytical formulas [34–36].

On the other hand, the Ultra Discretization (UD) procedure has been developed mainly in the field of soliton theory and cellular automaton (CA) theory [37–41]. Although the common discretization process discretizes independent variables, the UD procedure can discretize dependent variables. As a result, both independent and dependent variables become discrete variables. In other words, UD transforms discretized equations into their corresponding UD equations. In soliton theory, we can obtain the cellular automaton from the corresponding discretized soliton theory after UD procedure. In [40], it is shown that the corresponding integrable CA is obtained from Kortewegde Vries (KdV) soliton equation via Lotka-Volterra equation, using UD procedure. The key point of UD is that the UD procedure can be applied

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<sup>1</sup> Note added: After finishing our paper, we became aware of a recent paper done independently by Zhao et al.[43], in which the statistical properties of the MDS were studied. Although the starting point of the cavity analysis is similar, in their results they estimate the size of MDS by population dynamics simulations. In contrast, as shown later, we derive analytical solution for the size of the MDS.

only in the case that the original discretized equation does not have any minus operators.

By combining the cavity method and UD procedure, we solved for the first time the density of MDS problem analytically for any complex network. By cavity method and UD, we derived a combinatorial expression that allows us to identify the density of MDS by only using the degree distribution of the network, which is our main result. We then compare the results of the derived expression for density of MDS with the ILP solutions for regular, random and scale-free networks showing a fair agreement. Moreover, a simple formula is derived for random networks at the large degree limit.

## THEORETICAL RESULTS

### The Hamiltonian of a dominating set

A graph  $G = (V, E)$  is a set of nodes  $V$  and edges  $E$ . A Dominant Set (DS)  $S$  is defined to be a subset of  $V$ , where each node  $i \in V$  belongs to  $S$  or adjacent to an element of  $S$ . For each node  $i \in V$ , we define a binary function  $\sigma_i$  to be +1 if  $i \in S$ , otherwise 0. We call the node  $i$  occupied (resp. empty) if  $\sigma_i$  is +1 (resp. 0). The set of the adjacent nodes to node  $i$  is denoted by  $\partial i$ . We can then see that the constraint to define a DS is as follows:

$$\sigma_i + \sum_{j \in \partial i} \sigma_j \geq 1. \quad (1)$$

For each node  $i \in V$ , we define a binary function  $I_i$  to be +1 if and only if  $\sigma_i + \sum_{j \in \partial i} \sigma_j \geq 1$ , otherwise 0. A set  $S$  is an Minimum Dominating Set (MDS) if the size is smallest among all dominating sets (see Fig. 1).

Let us consider the following Hamiltonian function:

$$H(\sigma) = \sum_{i \in V} \sigma_i, \quad (2)$$

where  $\sigma = \{\sigma_i | i \in V\}$ . Then the partition function is given by

$$Z(\beta) = \sum_{\sigma} \left( \prod_{i \in V} I_i \right) \exp(-\beta H(\sigma)), \quad (3)$$

where the summation is taken over all configurations of  $\sigma$  and  $\beta$  is the inverse temperature.

## Cavity method analysis

In what follows, we apply the cavity method to derive the analytic formula for the density of MDS in complex networks. Note that the cavity approach has been used in a similar way to solve the maximal independent set problem [30]. First, we assume the graph  $G$  has tree structure and let  $\partial i \setminus j$  be the set of  $\partial i$  except for node  $j$  (see Fig. 2). Note also that the minimum degree of the graph should be two, otherwise some of  $\partial i \setminus j$  do not exist. Then, we can write  $\sigma_{i \rightarrow j} = \{\sigma_k | k \in \partial i \setminus j\}$ . Next, let  $\nu_{i \rightarrow j}(\sigma_i, \sigma_{i \rightarrow j})$  be the probability that the node  $i$  and  $\partial i \setminus j$  take value  $\sigma_i$  and  $\sigma_{i \rightarrow j}$ , respectively, and constraints  $I_i$  and  $I_j$  are not included:

$$\nu_{i \rightarrow j}(\sigma_i, \sigma_{i \rightarrow j}) = \frac{1}{Z_{i \rightarrow j}} \sum_{\sigma'} \left( \prod_{\alpha \neq i, j} I_\alpha \right) \exp(-\beta H(\sigma)), \quad (4)$$

where the first summation is taken over all configurations of  $\sigma' = \{\sigma_\beta | (\beta \neq i) \wedge (\beta \notin \partial i \setminus j) \wedge (\beta \in V)\}$ . The product for the constraint  $I_\alpha$  is taken over all nodes of  $V$  except for  $i, j$  (i.e.  $\alpha \in V$  and  $\alpha \neq i, j$ ) and  $Z_{i \rightarrow j}$  is the normalization constant given by

$$\begin{aligned} Z_{i \rightarrow j} &= \sum_{\sigma_i} \sum_{\sigma_{i \rightarrow j}} \sum_{\sigma'} \left( \prod_{\alpha \neq i, j} I_\alpha \right) \exp(-\beta H(\sigma)) \\ &= \sum_{\sigma} \left( \prod_{\alpha \neq i, j} I_\alpha \right) \exp(-\beta H(\sigma)). \end{aligned} \quad (5)$$

Eq. (4) can be written in a different way, which will be easier to compute. As shown in Fig. 3, we divide a graph into two subgraphs ( $A$  and  $B$ ) by cutting the edge  $(i, j)$  between node  $i$  and  $j$ . Let  $A$  be the set of all the nodes which belongs to the subgraph including  $i$ , and  $B$  be the set of all the nodes which belongs to the subgraph including  $j$ . Then, Eq. (4) can be transformed into

$$\nu_{i \rightarrow j}(\sigma_i, \sigma_{i \rightarrow j}) = \frac{1}{Z'_{i \rightarrow j}} \sum_{\sigma'_A} \left( \prod_{\alpha \neq i} I_\alpha \right) \exp(-\beta \sum_{\gamma \in A} \sigma_\gamma), \quad (6)$$

where the first summation is taken over all configurations of  $\sigma'_A = \{\sigma_\beta | (\beta \neq i) \wedge (\beta \notin \partial i \setminus j) \wedge (\beta \in A)\}$ . The product for the constraint  $I_\alpha$  is taken over all nodes of  $A$  except  $i$  (i.e.  $\alpha \in A$  and  $\alpha \neq i$ ) and  $Z'_{i \rightarrow j}$  is a normalization constant given by

$$\begin{aligned} Z'_{i \rightarrow j} &= \sum_{\sigma_i} \sum_{\sigma_{i \rightarrow j}} \sum_{\sigma'_A} \left( \prod_{\alpha \neq i} I_\alpha \right) \exp(-\beta \sum_{\gamma \in A} \sigma_\gamma) \\ &= \sum_{\sigma_A} \left( \prod_{\alpha \neq i} I_\alpha \right) \exp(-\beta \sum_{\gamma \in A} \sigma_\gamma), \end{aligned} \quad (7)$$

where the last summation is taken over all configurations of  $\sigma_A = \{\sigma_\beta | (\beta \in A)\}$ .

Then the following exact recursive equation can be derived:

$$\nu_{i \rightarrow j}(\sigma_i, \sigma_{i \rightarrow j}) \propto e^{-\beta \sigma_i} \prod_{k \in \partial i \setminus j} \sum_{\sigma_{k \rightarrow i}} I_k \nu_{k \rightarrow i}(\sigma_k, \sigma_{k \rightarrow i}). \quad (8)$$

This equation can be iteratively solved with its corresponding normalization constant.

Let  $\bar{\nu}(\sigma_i, m)$  be the summation of  $\nu_{i \rightarrow j}(\sigma_i, \sigma_{i \rightarrow j})$ , where the number of occupied neighbors  $\sigma_{i \rightarrow j}$  is  $m$ :

$$\bar{\nu}_{i \rightarrow j}(\sigma_i, m) = \sum_{\sum_{\alpha \in \partial i \setminus j} \sigma_\alpha = m} \nu_{i \rightarrow j}(\sigma_i, \sigma_{i \rightarrow j}). \quad (9)$$

Then, let  $r_1^{i \rightarrow j}$  be the probability that the node  $i$  is occupied in the cavity graph. Let  $r_{00}^{i \rightarrow j}$  be the probability that the node  $i$  and all the neighbors  $\sigma_{i \rightarrow j}$  are empty. Let  $r_0^{i \rightarrow j}$  be the probability that the node  $i$  is empty and at least one of the neighbors  $\sigma_{i \rightarrow j}$  are occupied.

Then, we can write:

$$r_1^{i \rightarrow j} = \sum_{m=0}^{k_i-1} \bar{\nu}_{i \rightarrow j}(1, m), \quad (10)$$

$$r_{00}^{i \rightarrow j} = \bar{\nu}_{i \rightarrow j}(0, 0), \quad (11)$$

$$r_0^{i \rightarrow j} = \sum_{m=1}^{k_i-1} \bar{\nu}_{i \rightarrow j}(0, m), \quad (12)$$

where  $k_i$  is the degree of node  $i$ . Here we note that  $r_1^{i \rightarrow j} + r_{00}^{i \rightarrow j} + r_0^{i \rightarrow j} = 1$ , because of probability normalization.

The above definitions lead to the following iterative equations:

$$r_1^{i \rightarrow j} = \frac{1}{N} e^{-\beta}, \quad (13)$$

$$r_{00}^{i \rightarrow j} = \frac{1}{N} \prod_{k \in \partial i \setminus j} r_0^{k \rightarrow i}, \quad (14)$$

$$r_0^{i \rightarrow j} = \frac{1}{N} \left\{ \prod_{k \in \partial i \setminus j} (1 - r_{00}^{k \rightarrow i}) - \prod_{k \in \partial i \setminus j} r_0^{k \rightarrow i} \right\}, \quad (15)$$

where  $N$  is the normalization constant given by

$$N = e^{-\beta} + \prod_{k \in \partial i \setminus j} (1 - r_{00}^{k \rightarrow i}). \quad (16)$$

### Ultra-Discretization (UD) procedure

We note that until now we are considering the problem of an DS, which is treated as finite temperature problem ( $\beta$  is finite) in the context of statistical mechanics. To address the

minimum dominating set (MDS) problem, we have to consider the zero-temperature limit ( $\beta \rightarrow \infty$ ) which gives the ground energy state of the Hamiltonian shown in Eq. (2). To solve the equations associated to the zero-temperature limit, we can use an Ultra-Discretization (UD) procedure [40].

Equation	independent variable	dependent variable
(i) Continuous equation for $x(t)$	$t$ : real value	$x(t)$ : real value
(ii) Discretized equation for $x_n$	$n$ : integer	$x_n$ : real value
(iii) Ultra- Discretized (UD) equation for $X_n$	$n$ : integer	$X_n$ : integer

TABLE I. Discretization procedure changes the equation type from (i) to (ii) and Ultra-Discretization procedure transforms the equation type from (ii) to (iii).

Discretization is a well-known method to discretize independent variable in continuous theory such as differential equation (see Table 1 from (i) to (ii)). UD can go further and aims to discretize the dependent variable in the discretized equation (from (ii) to (iii)). As a result, in the transformed UD equation (iii), both independent and dependent variables are discretized (i.e. both are integer variables). The key formula of UD, which transforms the equation type from (ii) to (iii) is

$$\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \log(e^{\beta X} + e^{\beta Y}) = \max(X, Y). \quad (17)$$

When the discretized equation (ii) has no subtraction operator, we can transform it into the corresponding UD equation (iii) by replacing  $x = e^{\beta X}$  and  $y = e^{\beta Y}$  and taking limit  $\beta \rightarrow \infty$ . Here,  $x$  and  $y$  belong to discretized equation (ii) and  $X$  and  $Y$  belong to UD equation (iii). The operator in the original discretized equation (ii) is transformed in the UD equation (iii) as follows:

$$x \times y \rightarrow X + Y, \quad (18)$$

$$x/y \rightarrow X - Y, \quad (19)$$

$$x + y \rightarrow \max(X, Y). \quad (20)$$

Here we remark that in order to obtain the UD equation (iii), it is necessary to be able to remove any minus operator in the original discretized equation (ii).

In order to ultra-discretize the previous Eqs. (13), (14) and (15), we make them consist of only plus, multiplication and division operators, avoiding minus operators. By simple

computation, we have

$$\prod_{k \in \partial i \setminus j} (1 - r_{00}^{k \rightarrow i}) = \prod_{k \in \partial i \setminus j} (r_0^{k \rightarrow i} + r_1^{k \rightarrow i}) \quad (21)$$

and

$$\prod_{k \in \partial i \setminus j} (1 - r_{00}^{k \rightarrow i}) - \prod_{k \in \partial i \setminus j} r_0^{k \rightarrow i} = \sum_{1 \leq m_1 + \dots + m_n \leq n} r_{m_1}^{k_1 \rightarrow i} r_{m_2}^{k_2 \rightarrow i} \dots r_{m_n}^{k_n \rightarrow i}, \quad (22)$$

where  $n$  is the number of elements of  $\partial i \setminus j$ , and  $m_p = 0$  or  $1$  ( $p = 1, 2, 3, \dots, n$ ).

By inserting Eqs. (21) and (22) into Eqs. (13), (14) and (15), we have

$$r_1^{i \rightarrow j} = \frac{e^{-\beta}}{e^{-\beta} + \prod_{k \in \partial i \setminus j} (r_0^{k \rightarrow i} + r_1^{k \rightarrow i})}, \quad (23)$$

$$r_{00}^{i \rightarrow j} = \frac{\prod_{k \in \partial i \setminus j} r_0^{k \rightarrow i}}{e^{-\beta} + \prod_{k \in \partial i \setminus j} (r_0^{k \rightarrow i} + r_1^{k \rightarrow i})}, \quad (24)$$

$$r_0^{i \rightarrow j} = \frac{\sum_{1 \leq m_1 + \dots + m_n \leq n} r_{m_1}^{k_1 \rightarrow i} r_{m_2}^{k_2 \rightarrow i} \dots r_{m_n}^{k_n \rightarrow i}}{e^{-\beta} + \prod_{k \in \partial i \setminus j} (r_0^{k \rightarrow i} + r_1^{k \rightarrow i})}. \quad (25)$$

Here we remark that the above derived equations consist only of three operators (plus, multiplication and division), which is suitable for the ultra-discretization.

Here, we then replace the following three variables as follows:

$$r_1^{i \rightarrow j} = e^{\beta R_1^{i \rightarrow j}}, \quad (26)$$

$$r_{00}^{i \rightarrow j} = e^{\beta R_{00}^{i \rightarrow j}}, \quad (27)$$

$$r_0^{i \rightarrow j} = e^{\beta R_0^{i \rightarrow j}}, \quad (28)$$

where  $R_1^{i \rightarrow j}$ ,  $R_{00}^{i \rightarrow j}$  and  $R_0^{i \rightarrow j}$  are variables in UD system.

After inserting (26), (27), (28) into (23), (24), (25) and taking zero-temperature limit  $\beta \rightarrow \infty$ , Eqs. (23), (24) and (25) are transformed into

$$R_1^{i \rightarrow j} = -1 - \max(-1, \sum_{k \in \partial i \setminus j} \max(R_0^{k \rightarrow i}, R_1^{k \rightarrow i})), \quad (29)$$

$$R_{00}^{i \rightarrow j} = \sum_{k \in \partial i \setminus j} R_0^{k \rightarrow i} - \max(-1, \sum_{k \in \partial i \setminus j} \max(R_0^{k \rightarrow i}, R_1^{k \rightarrow i})), \quad (30)$$

$$R_0^{i \rightarrow j} = \max_{1 \leq m_1 + \dots + m_n \leq n} (R_{m_1}^{k_1 \rightarrow i} + R_{m_2}^{k_2 \rightarrow i} + \dots + R_{m_n}^{k_n \rightarrow i}) - \max(-1, \sum_{k \in \partial i \setminus j} \max(R_0^{k \rightarrow i}, R_1^{k \rightarrow i})). \quad (31)$$

Eq. (23), (24), (25) (or Eq. (29), (30), (31)) are very difficult to solve, because every edge direction has three variables and three associated equations. Therefore, in order to avoid this high complexity, we use a coarse-grained method.



Let  $p_k$  be the degree distribution of the network which gives the probability to find nodes with degree  $k$  and  $\langle k \rangle = \sum_k k p_k$  be the average degree of the network. The excess degree distribution is given by  $q_k = (k+1)p_{k+1}/\langle k \rangle$ , that is the probability to find that a neighbor node has degree  $k$ .

Let us assume that the network is enough large. Each  $r_1^{i \rightarrow j}$  and  $r_0^{i \rightarrow j}$  values are assigned to the edge direction from  $i$  to  $j$ . The opposite edge direction gets the values from  $r_1^{j \rightarrow i}$  and  $r_0^{j \rightarrow i}$ .  $r_0^{i \rightarrow j}$  is not independent variable because of the normalization. Let  $P(r_1, r_0)$  be the probability density function of  $r_1^{i \rightarrow j}$ ,  $r_0^{i \rightarrow j}$ .

Then we have the coarse-grained equation (cavity mean field equation) for (23) and (25) as follows:

$$\begin{aligned}
P(r_1, r_0) = & \sum_{k=1}^{\infty} q_k \int \prod_{l=1}^k dr_1^l dr_0^l P(r_1^l, r_0^l) \\
& \times \delta(r_1 - \frac{e^{-\beta}}{e^{-\beta} + \prod_{l=1}^k (r_0^l + r_1^l)}) \\
& \times \delta(r_0 - \frac{\sum_{1 \leq m_1 + \dots + m_k \leq k} r_{m_1}^1 r_{m_2}^2 \dots r_{m_k}^k}{e^{-\beta} + \prod_{l=1}^k (r_0^l + r_1^l)}). \tag{32}
\end{aligned}$$

We transform the probability density function by variables transformation (26) and (28) as follows:

$$P(r_1, r_0) dr_1 dr_0 = \bar{P}(R_1, R_0) dR_1 dR_0. \tag{33}$$

Then, we have

$$\begin{aligned}
\bar{P}(R_1, R_0) = & \sum_{k=1}^{\infty} q_k \int \prod_{l=1}^k dR_1^l dR_0^l \bar{P}(R_1^l, R_0^l) \\
& \times \delta(r_1 - \frac{1}{\beta} \log \frac{e^{-\beta}}{e^{-\beta} + \prod_{l=1}^k (e^{\beta R_0^l} + e^{\beta R_1^l})}) \\
& \times \delta(r_0 - \frac{1}{\beta} \log \frac{\sum_{1 \leq m_1 + \dots + m_k \leq k} e^{\beta R_{m_1}^1} e^{\beta R_{m_2}^2} \dots e^{\beta R_{m_k}^k}}{e^{-\beta} + \prod_{l=1}^k (e^{\beta R_0^l} + e^{\beta R_1^l})}). \tag{34}
\end{aligned}$$

Taking UD limit (zero temperature)  $\beta \rightarrow \infty$ , we have the ultra-discretization version of cavity equation:

$$\begin{aligned}
\bar{P}(R_1, R_0) = & \sum_{k=1}^{\infty} q_k \int \prod_{l=1}^k dR_1^l dR_0^l \bar{P}(R_1^l, R_0^l) \\
& \times \delta(R_1 + 1 + \max(-1, \sum_{l=1}^k \max(R_0^l, R_1^l))) \\
& \times \delta(R_0 - \max_{1 \leq m_1 + \dots + m_k \leq k} (R_{m_1}^1 + R_{m_2}^2 + \dots + R_{m_k}^k) + \max(-1, \sum_{l=1}^k \max(R_0^l, R_1^l))). \tag{35}
\end{aligned}$$

Next, we will solve this equation. Eqs. (29), (30), (31) imply that  $R_1$  and  $R_0$  takes integer values, since  $R_1$  and  $R_0$  at the boundary of network takes integer values. Furthermore, considering the probability conservation, Eqs. (26), (28) imply that  $R_1$  and  $R_0$  takes value 0 or negative integer. By considering Eq. (29), firstly, we can see that  $R_1^{i \rightarrow j}$  takes value only 0 or  $-1$ . Secondly, if  $R_1^{i \rightarrow j}$  is  $-1$ , then for each  $k \in \partial i \setminus j$ , one of  $R_0^{k \rightarrow i}$  or  $R_1^{k \rightarrow i}$  takes value 0. In this case ( $R_1^{i \rightarrow j} = -1$ ), from Eq. (31),  $R_0^{i \rightarrow j}$  takes value 0 or  $-1$ . Therefore, we can set the distribution  $\bar{P}(R_1, R_0)$  as follows:

$$\bar{P}(R_1, R_0) = a\delta(R_1 + 1)\delta(R_0) + b\delta(R_1 + 1)\delta(R_0 + 1) + \sum_{n=0}^{\infty} c_n\delta(R_1)\delta(R_0 + n), \quad (36)$$

where  $a + b + \sum_{n=0}^{\infty} c_n = 1$ .

Inserting (36) into the cavity equation (35), we have

$$a = \sum_{k=1}^{\infty} q_k((1-b)^k - a^k), \quad (37)$$

$$b = \sum_{k=1}^{\infty} q_k a^k, \quad (38)$$

$$c_{m-1} = \sum_{k=m}^{\infty} q_k ({}_k C_m) b^m (1-b)^{k-m} \quad (m = 1, 2, 3, \dots). \quad (39)$$

Once the degree distribution  $p_k$  is given, we can determine  $a$ ,  $b$ ,  $c_n$  ( $n = 0, 1, 2, \dots$ ).

Here, we need the average energy of the Hamiltonian (2), which can be identified as the average number of all DS configurations. After taking zero temperature limit  $\beta \rightarrow \infty$ , we will obtain the analytical formula for the density of MDS.

The average energy can be computed by  $\langle H \rangle = -\frac{\partial}{\partial \beta} \log Z$ , where the partition function is shown in Supplementary Information. A generic expression for density is given by

$$\begin{aligned} \rho &= \frac{\langle H \rangle}{|V|} \\ &= \sum_{k=2}^{\infty} p_k \int \prod_{l=1}^k dr_1^l dr_0^l P(r_1^l, r_0^l) \frac{e^{-\beta}}{e^{-\beta} + \prod_{l=1}^k (r_0^l + r_{00}^l) - \prod_{l=1}^k r_0^l}. \end{aligned} \quad (40)$$

This equation, however, cannot be ultra-discretized because of the minus operator, and without being ultra-discretized, analytical solution cannot be obtained. Therefore, we avoid minus operator by inserting Eqs. (21) and (22), which leads to the following result:

$$\rho = \sum_{k=2}^{\infty} p_k \int \prod_{l=1}^k dr_1^l dr_0^l P(r_1^l, r_0^l) \frac{e^{-\beta}}{e^{-\beta} + \sum_{1 \leq m_1 + \dots + m_k \leq k} (r_{m_1}^1 \dots r_{m_k}^k)}. \quad (41)$$

After taking zero temperature limit  $\beta \rightarrow \infty$ , we obtain

$$\rho = \lim_{\beta \rightarrow \infty} \sum_{k=2}^{\infty} p_k \int \prod_{l=1}^k dR_1^l dR_0^l P(R_1^l, R_0^l) \frac{e^{-\beta}}{e^{-\beta} + \sum_{1 \leq m_1 + \dots + m_k \leq k} e^{\beta(R_{m_1}^1 + R_{m_2}^2 + \dots + R_{m_k}^k)}} \quad (42)$$

By inserting (36) into this equation, we finally obtain

$$\begin{aligned} \rho = & \sum_{k=2}^{\infty} p_k \left[ 1 - (1-b)^k - kb(1-b)^{k-1} + a^k \frac{1}{k+1} \right. \\ & + \sum_{p+q+r=k-1} \frac{k!}{p!r!s!} a^p b (c_0)^r (1-b-c_0)^s \frac{1}{1+2^{r+1}} \\ & \left. + \sum_{p+r=k-1} \frac{k!}{p!r!} a^p b (c_0)^r \left( \frac{1}{1+2^{r+1}} - \frac{1}{2^{r+1}} \right) \right]. \end{aligned} \quad (43)$$

More simply, we transform the previous equation into

$$\begin{aligned} \rho = & \sum_{k=2}^{\infty} p_k \left[ 1 - (1-b)^k - kb(1-b)^{k-1} + a^k \frac{1}{k+1} \right. \\ & \left. + \sum_{r=0}^{k-1} \frac{k!}{(k-r-1)!r!} b c_0^r \times \left\{ (1-b-c_0)^{k-r-1} \frac{1}{1+2^{r+1}} - a^{k-r-1} \left( \frac{1}{1+2^{r+1}} - \frac{1}{2^{r+1}} \right) \right\} \right]. \end{aligned} \quad (44)$$

Eq. (44) is our main result. Using this equation, we can analytically compute the density of MDS from any degree distribution  $p_k$ . More concretely, we can summarize the procedure as follows. Once the degree density function  $p_k$  is given, we can easily compute the excess degree density function  $q_k$ . Then, by solving (37), (38) and (39), we obtain  $a, b, c_n$  ( $n = 0, 1, 2, \dots$ ). Finally, inserting the value  $a, b, c_n$  ( $n = 0, 1, 2, \dots$ ) into the above equation (44), we obtain the density of MDS.

We note that when we consider random network with average degree  $z$  as a special case, we can derive the simple expression  $\rho = 1/z$  by using large average degree limit approximation ( $z \rightarrow \infty$ ) (See supplementary Information).

## COMPUTATIONAL RESULTS

Here we performed computer simulations to examine the theoretical results (44) obtained using cavity method. First, we consider regular and random networks constructed with a variety of average degree values (see Fig. 4 (a) and (b)). The results show that cavity method predictions are in excellent agreement with ILP solutions.

Next, we examine the case of scale-free networks. We first generated samples of synthetic scale-free networks with a variety of scaling exponent  $\gamma$  and average degree  $\langle k \rangle$  using the Havel-Hakimi algorithm with random edge swaps (HMC). All samples were generated with a size of  $N = 5000$  nodes. We investigated two different cases. We constructed a set of scale-free network samples with natural cut-off  $k_c = N - 1$  and another set with structural cut-off  $k_c = \sqrt{\langle k \rangle N}$ . The minimum degree is  $k_{min} = 2$  in both cases. Fig. 5 shows the results for natural cut-off (i.e. no structural cut-off is considered). The dependence of the MDS density  $\rho$  as a function of the average degree  $\langle k \rangle$  shows a good agreement with the cavity method analytical predictions (44), in particular when  $\gamma$  increases (see Figs. 5 (c)-(e)). By increasing the average degree, the MDS density  $\rho$  decreases. For small values of  $\gamma$ , the predictions of the cavity method deviates from the ILP solutions when average degree increases (see Fig. 5(b)). The reason is because in this case, the network tends to have hubs with very high degree. While these hubs are still visible to ILP method, they are not observed by the cavity method. It is well-known that cavity method addresses better homogeneous networks than extremely inhomogeneous networks. On the other hand, by examining the function of MDS density  $\rho$  versus  $\gamma$ , we clearly observe the influence of the average degree (see Fig. 5(a)). Moreover, in absence of structural cut-off, for high average degree networks, the MDS density  $\rho$  for ILP decreases faster than the solution for cavity method when  $\gamma$  decreases.

We have also considered the case of structural cut-off when constructing finite artificial scale-free networks to address the finite-size effect and eliminate degree correlations. The computer simulations on scale-free networks with structural cut-off shows a different picture (see Fig. 6(a)-(e)). The MDS density  $\rho$  does not significantly changes when  $\gamma$  decreases and remains constant along all the range of  $\gamma$  values (see Fig. 6(a)). Moreover, when structural cut-off is considered, the agreement between cavity method and ILP results becomes more evident for any value of  $\gamma$  and average degree (see Fig. 6 (b)-(e)). The reason is because the network tends to be more homogeneous when some hubs with extremely high-degree are knocked out by the structural cut-off.

## CONCLUSION

Domination is not only one of the most active research areas in graph theory but also has found abundant real-world applications in many different fields, from engineering to social and natural sciences. With the recent years expansion of networks as data representation framework, domination techniques may provide a rich set of tools to face current network problems in society and nature.

In this work, by using the cavity method and the ultra-discretization procedure, we solved for the first time the MDS problem analytically and derived a combinatorial equation whose computation is easier than that of ILP. By only using the degree distribution of a network as an input information, we can compute the density of an MDS and investigate any dependence with respect to other network variables without using assistance of any complex optimization methods such as ILP or DP.

The present analysis may allow a variety of rich extensions such as computing the corresponding analytical expression for MDS density in directed and bipartite networks.

## ACKNOWLEDGEMENTS

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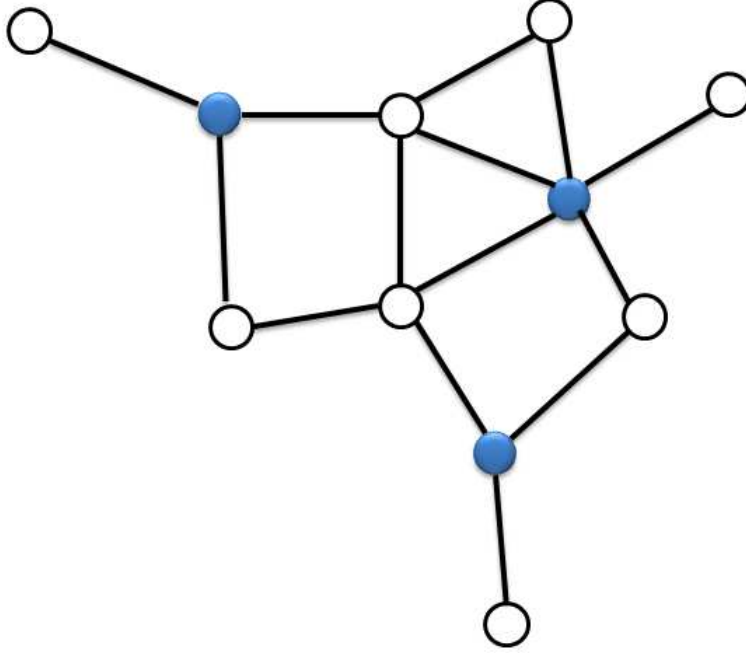


FIG. 1. Illustration of an MDS. Filled nodes belong to the MDS.

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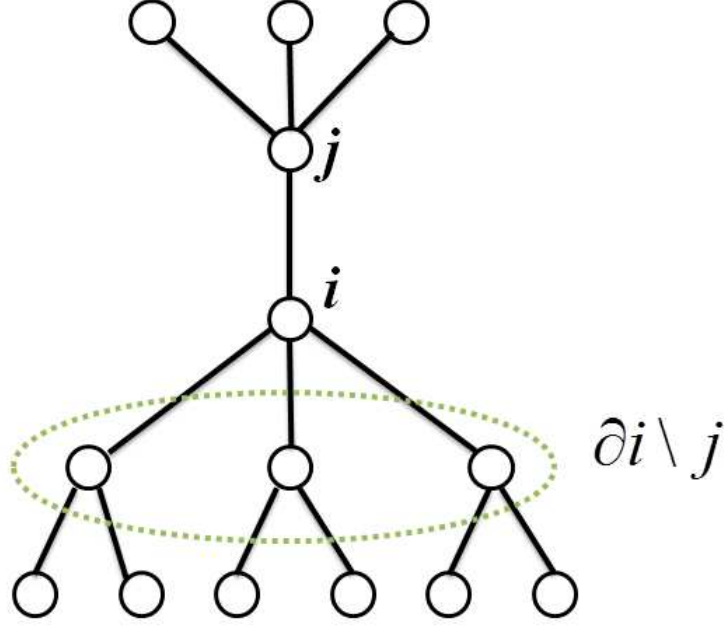


FIG. 2. An example of a tree graph. The highlighted nodes  $\partial i \setminus j$  indicate the set of nodes adjacent to  $i$  except for node  $j$ .

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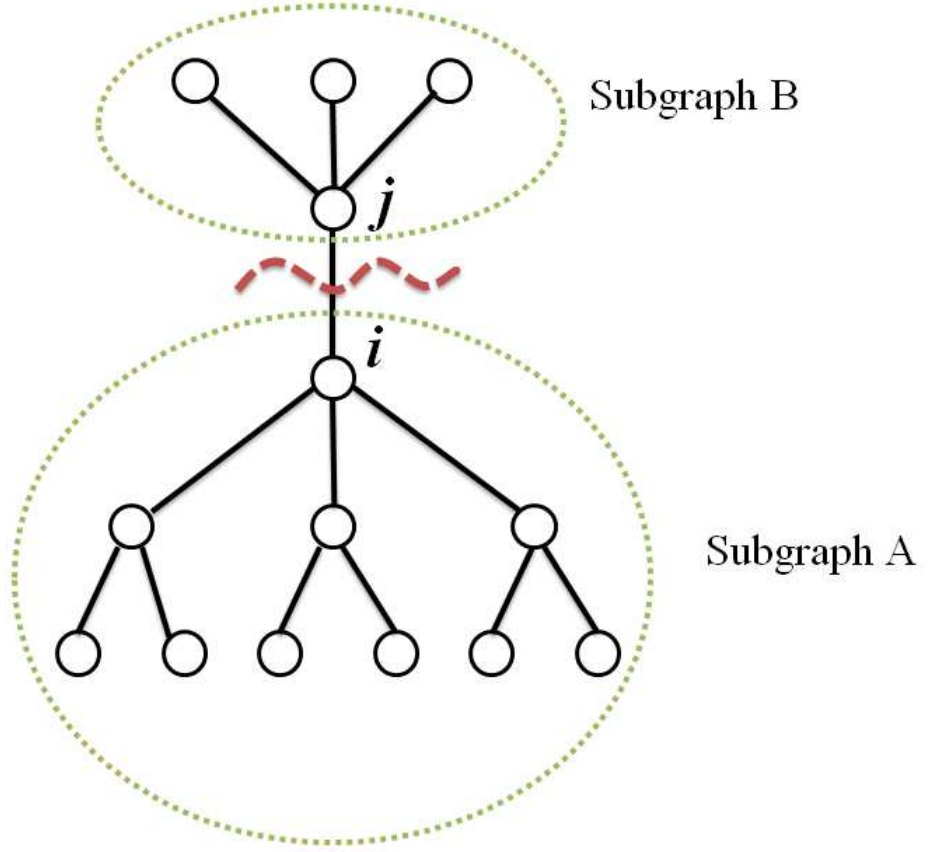


FIG. 3. Two subgraphs ( $A$  and  $B$ ) are obtained by cutting an edge  $(i, j)$ . Note that subgraph  $A$  and  $B$  includes nodes  $i$  and  $j$ , respectively.

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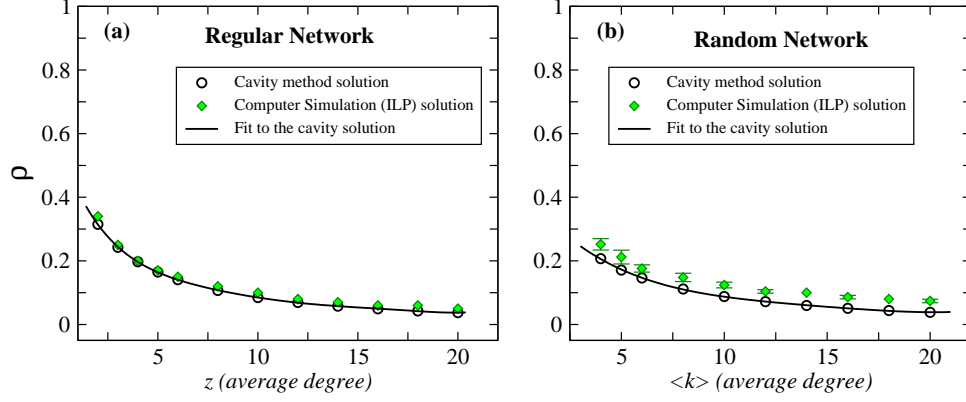


FIG. 4. Comparison of the cavity method and ILP results for the MDS density  $\rho$  in regular (a) and random (b) networks constructed with a variety of average degree values. The results are averaged using five network samples. For cavity method the standard deviation (SD) is smaller than symbol. For ILP the SD is shown for each symbol.

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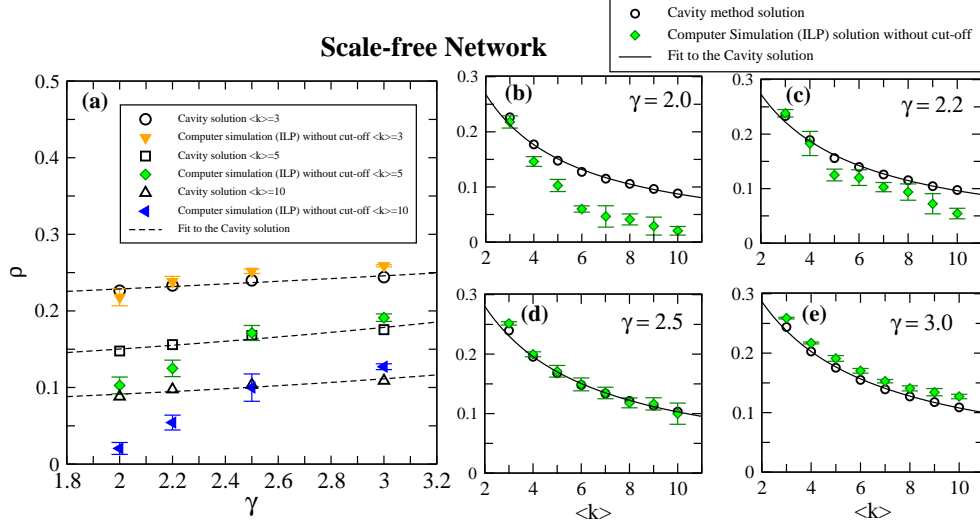


FIG. 5. Comparison of the cavity method and ILP results for the MDS density  $\rho$  in samples of synthetic scale-free networks generated without structural cut-off  $k_c = N - 1$ .  $\rho$  as a function of the scaling exponent  $\gamma$  (a) and average degree  $\langle k \rangle$  (b-d) are shown in figure. The results are averaged using five network samples with a size of  $N = 5000$  nodes. For cavity method the standard deviation (SD) is smaller than symbol. For ILP the SD is shown for each symbol.

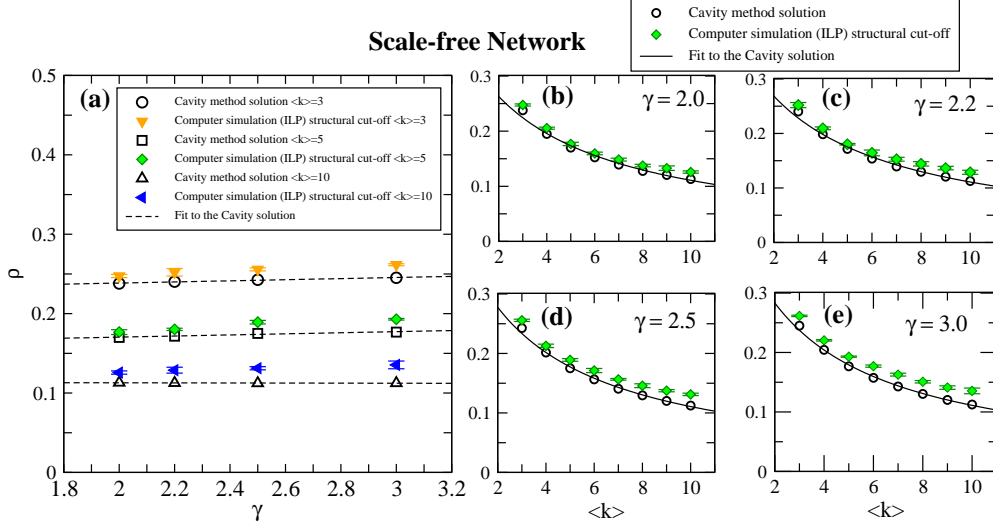


FIG. 6. Comparison of the cavity method and ILP results for the MDS density  $\rho$  in samples of synthetic scale-free networks generated with structural cut-off  $k_c = \sqrt{\langle k \rangle N}$ .  $\rho$  as a function of the scaling exponent  $\gamma$  (a) and average degree  $\langle k \rangle$  (b-d) are shown in figure. The results are averaged using five network samples with a size of  $N = 5000$  nodes. For cavity method the standard deviation (SD) is smaller than symbol. For ILP the SD is shown for each symbol.

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# Supplementary Information

## Analytical Solution for the Size of the Minimum Dominating Set in Complex Networks

*Jose C. Nacher and Tomoshiro Ochiai*

### Contents

I. Derivation of the partition function of the Hamiltonian	1
II. A simple analytic expression for MDS in random networks	2

### I. DERIVATION OF THE PARTITION FUNCTION OF THE HAMILTONIAN

In this section, we will derive the partition function of the Hamiltonian (see Eq. (3) in main text), as in [30,42].

By removing node  $a$ , we define cavity partition function  $Z_a$  by

$$Z_a = \prod_{b \in \partial a} Z'_{b \rightarrow a}. \quad (1)$$

Similarly, by removing an edge  $(ab)$ , we define cavity partition function  $Z_{(ab)}$  by

$$Z_{(ab)} = Z'_{a \rightarrow b} Z'_{b \rightarrow a}. \quad (2)$$

Let us define cavity free energy  $\Delta f_a$  by

$$\begin{aligned} e^{-\beta \Delta f_a} &\equiv \frac{Z}{Z_a} \\ &= \sum_{\sigma_a} \sum_{\{\sigma_b | b \in \partial a\}} \sum_{\{\sigma_{b \rightarrow a} | b \in \partial a\}} e^{-\beta \sigma_a} I_a \prod_{b \in \partial a} I_b \nu_{b \rightarrow a}(\sigma_b, \sigma_{b \rightarrow a}). \end{aligned} \quad (3)$$

Here the last equality holds after some computation. We then define cavity free energy  $\Delta f_{(ab)}$  by

$$\begin{aligned} e^{-\beta \Delta f_{(ab)}} &\equiv \frac{Z}{Z_{(ab)}} \\ &= \sum_{\sigma_a} \sum_{\sigma_{a \rightarrow b}} \sum_{\sigma_b} \sum_{\sigma_{b \rightarrow a}} I_a I_b \nu_{a \rightarrow b}(\sigma_a, \sigma_{a \rightarrow b}) \nu_{b \rightarrow a}(\sigma_b, \sigma_{b \rightarrow a}). \end{aligned} \quad (4)$$

Furthermore, we can transform (3) and (4) as follows:

$$\begin{aligned}\frac{Z}{Z_a} &= e^{-\beta} + \prod_{b \in \partial a} (1 - r_{00}^{b \rightarrow a}) - \prod_{b \in \partial a} r_0^{b \rightarrow a} \\ &= e^{-\beta} + \prod_{b \in \partial a} (r_0^{b \rightarrow a} + r_1^{b \rightarrow a}) - \prod_{b \in \partial a} r_0^{b \rightarrow a},\end{aligned}\quad (5)$$

and

$$\begin{aligned}\frac{Z}{Z_{(ab)}} &= r_1^{a \rightarrow b} r_1^{b \rightarrow a} + r_0^{a \rightarrow b} r_0^{b \rightarrow a} + r_1^{a \rightarrow b} (r_0^{b \rightarrow a} + r_{00}^{b \rightarrow a}) + (r_0^{a \rightarrow b} + r_{00}^{a \rightarrow b}) r_1^{b \rightarrow a} \\ &= r_1^{a \rightarrow b} r_1^{b \rightarrow a} + r_0^{a \rightarrow b} r_0^{b \rightarrow a} + r_1^{a \rightarrow b} (1 - r_1^{b \rightarrow a}) + (1 - r_1^{a \rightarrow b}) r_1^{b \rightarrow a}.\end{aligned}\quad (6)$$

When the graph is a tree, we have  $|V| = |E| + 1$ , where  $|V|$  and  $|E|$  is the number of nodes  $V$  and edges  $E$ , respectively. Then, the partition function can be decomposed as follows:

$$Z = e^{-\beta N f} = \prod_{a \in V} \frac{Z}{Z_a} \prod_{(ab) \in E} \frac{Z_{(ab)}}{Z}.\quad (7)$$

By taking logarithm on the previous expression, we obtain

$$\begin{aligned}\log Z &= \sum_{a \in V} \log(e^{-\beta} + \prod_{b \in \partial a} (r_0^{b \rightarrow a} + r_1^{b \rightarrow a}) - \prod_{b \in \partial a} r_0^{b \rightarrow a}) \\ &\quad - \sum_{(ab) \in E} \log(r_1^{a \rightarrow b} r_1^{b \rightarrow a} + r_0^{a \rightarrow b} r_0^{b \rightarrow a} + r_1^{a \rightarrow b} (1 - r_1^{b \rightarrow a}) + (1 - r_1^{a \rightarrow b}) r_1^{b \rightarrow a}).\end{aligned}\quad (8)$$

Using a coarse-grained approximation, we obtain

$$\begin{aligned}\log Z &= |V| \sum_{k=2}^{\infty} p_k \int \prod_{l=1}^k dr_1^l dr_0^l P(r_1^l, r_0^l) \\ &\quad \times \log(e^{-\beta} + \prod_{l=1}^k (r_0^l + r_1^l) - \prod_{l=1}^k r_0^l) \\ &\quad - |E| \int \prod_{l=1}^2 dr_1^l dr_0^l P(r_1^l, r_0^l) \log(r_1^1 r_1^2 + r_0^1 r_0^2 + r_1^1 (1 - r_1^2) + (1 - r_1^1) r_1^2).\end{aligned}\quad (9)$$

## II. A SIMPLE ANALYTIC EXPRESSION FOR MDS IN RANDOM NETWORKS

Eq. (44) in main text provides us an analytical tool to compute the density of MDS for any kind of network. It may be possible, however, to obtain examine the behavior of this equation for specific network structures using some approximations. Below we derived the approximated analytical expression for the random network characterized with a Poisson degree distribution.

First, the density of the MDS can be evaluated using the following inequality:

$$\sum_{k=2}^{\infty} p_k [1 - (1-b)^k - kb(1-b)^{k-1} + a^k \frac{1}{k+1}] < \rho < \sum_{k=2}^{\infty} p_k [1 - (1-b)^k + a^k \frac{1}{k+1}]. \quad (10)$$

As a rough approximation, we set

$$\rho = \sum_{k=0}^{\infty} p_k [1 - (1-b)^k]. \quad (11)$$

Here we start the summation from  $k = 0$  instead of  $k = 2$  as an approximation. This approximation is good if the average degree is enough large. Let us define generating functions as follows:

$$G(x) = \sum_{k=0}^{\infty} p_k x^k, \quad (12)$$

$$H(x) = \sum_{k=0}^{\infty} q_k x^k. \quad (13)$$

Then, Eqs. (37-39) in main text can be rewritten as follows:

$$a = H(1-b) - H(a), \quad (14)$$

$$b = H(a), \quad (15)$$

$$\rho = 1 - G(1-b). \quad (16)$$

We use a Poisson distribution  $p_k = \frac{e^{-z} z^k}{k!}$ . Then we have  $q_k = \frac{e^{-z} z^k}{k!}$ . Using this distribution, we get  $H(x) = G(x) = e^{z(x-1)}$ . Inserting these into (14), (15) and (16), we get

$$a = e^{-zb} - e^{z(a-1)}, \quad (17)$$

$$b = e^{z(a-1)}, \quad (18)$$

$$\rho = 1 - e^{-zb}. \quad (19)$$

Here we derive the simple formula for the density of MDS by using the approximation in  $z \rightarrow \infty$ . From Eq.(17) and (18), we get

$$1 - a \sim b(z+1) \sim bz, \quad (20)$$

where we use the fact that  $bz$  is small, since we know that  $bz$  is small in numerical results.

In the same way, we get

$$\rho \sim bz. \quad (21)$$

Inserting Eq.(20) and (21) into (18), we get

$$b \sim e^{-bz^2} = e^{-\rho z} \sim 1 - \rho z, \quad (22)$$

where we use  $\rho z$  is small, since we know that  $\rho z$  is small in the simulated result in  $z \rightarrow \infty$ . From Eq.(21) and (22), we obtain

$$\rho \sim \frac{z}{1+z^2} \sim \frac{1}{z}. \quad (23)$$

This result shows that a high density of links implies a low MDS density. This inverse functional dependence with average degree is also observed in cavity method and ILP solutions shown in Fig. 4b.